EDGEWOOD
CHEMICAL BIOLOGICAL CENTER

U.S. ARMY RESEARCH, DEVELOPMENT AND ENGINEERING COMMAND

ECBC-TR-461

EVALUATION OF AHURA'S FIRSTDEFENDER HANDHELD CHEMICAL IDENTIFIER

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January 2006

ABERDEEN PROVING GROUND, MD 21010-5424

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*	2. REPORT TYPE	3. DATES COVERED *(From - To)*
XX-01-2006	Final	Apr 2005-May 2005

4. TITLE AND SUBTITLE
Evaluation of Ahura's FirstDefender Handheld Chemical Identifer

5a. CONTRACT NUMBER

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)
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5d. PROJECT NUMBER
0525T

5e. TASK NUMBER

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) AND ADDRESS(ES)
DIR, ECBC, ATTN: AMSRD-ECB-RT-PT, APG, MD 21010-5424
EAI Corporation, 1308 Continental Drive, Suite J, Abingdon, MD 21009
Ahura Corporation, 46 Jonspin Road, Wilmington, MA 01887

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)
Ahura Corporation, 46 Jonspin Road, Wilmington, MA 01887

10. SPONSOR/MONITOR'S ACRONYM(S)

11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION / AVAILABILITY STATEMENT
Approved for public release; distribution is unlimited.

13. SUPPLEMENTARY NOTES

14. ABSTRACT

The handheld Raman spectrometer for point detection of chemicals developed by Ahura Corporation was tested using chemical warfare agents (CWAs). The device was assessed for its capacity to detect and identify liquid through sealed glass containers in a completely non-contact, non-destructive manner. The CWAs tested included the following: mustard (HD), nitrogen mustard (HN1 and HN3), VX, tabun (GA), sarin (GB), and lewisite (L). Detection characteristics were examined for neat agents, as well as detection in the presence of interferences (JP8 jet fuel, aqueous film forming foam, Windex, and floor wax) at various concentrations.

15. SUBJECT TERMS

VX	Soman	Handheld detectors	Chemical warfare agents (CWA)
Tabun (GA)	Mustard (HD)	Interference testing	
Sarin (GB)	Lewisite (L)	Raman spectrometer	

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			Sandra J. Johnson
U	U	U	UL	53	19b. TELEPHONE NUMBER *(include area code)* 410-436-2914

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PREFACE

The work described in this report was authorized under Project No. 0525T and performed in conjunction with Ahura Corporation. The work was started in April 2005 and completed in May 2005.

The use of either trade or manufacturers' names in this report does not constitute an official endorsement of any commercial products.

This report has been approved for public release. Registered users should request additional copies from the Defense Technical Information Center; unregistered users should direct such requests to the National Technical Information Service.

Acknowledgments

The authors acknowledge Fredrick C. Baldauf, (ECBC) for his assistance in performing agent testing; and Terri L. Longworth (ECBC) for her assistance in test planning, acquisition, and review.

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1. INTRODUCTION

1.1 Background.

The rapid identification of potentially hazardous materials such as explosives, unknown chemicals, narcotics, or toxic industrial chemicals is becoming increasingly critical for military teams, emergency response teams, and other homeland security operations. Currently deployed bulk identification techniques are only man-portable and most require actually sampling or handling of the material of interest. Many of these tools are also far from the ruggedness and robustness needed in the field.

Raman spectroscopy is a technique which has been validated for rapid identification of chemicals, explosives, and narcotics.[1] As a laser scattering technique, Raman spectroscopy allows "line-of-sight' interrogation of samples through clear packaging or containers. Various toxic chemicals, chemical weapons, narcotics, and other unidentified potentially hazardous substances can be analyzed in glass vials, or plastic bags; greatly reducing the possibility of evidence corruption, cross contamination, or risk to response personnel.

Ahura Corporation (Appendix A) has developed a handheld (~ 4 lb) and rugged Raman chemical identification system. The handheld is fully self-contained, performs chemical analysis on board, and renders a probabilistic based result. The handheld allows the rapid (10's of seconds) identification of an unknown substance (solid, liquid, powder) in a nondestructive manner. This report provides the data and the respective analysis obtained during testing at the Applied Testing Team of RDECOM (AMSRD-ECB-RT-AT) at the U.S. Army Edgewood Chemical and Biological Center (ECBC) during Spring, 2005. The system is environmentally robust and has passed a subset of MIL STD 810F tests.

1.2 Objective and Scope.

The objective of this evaluation is to assess the general characteristics of the instrument and its ability to detect and identify the presence of chemical warfare (CW) agents in liquid form. Agent testing encompassed tabun (GA), sarin (GB), soman (GD), cyclosarin (GF), mustard (HD), VX, nitrogen mustard (HN1 and HN3) and lewisite (L). These agents were tested neat, as well as in mixtures with JP8 jet fuel, Windex, aqueous film forming foam (AFFF), and floor wax at a range of concentrations. As it is clearly desirable to avoid contact with these agents in routine field use, all measurements were made with the liquid samples sealed in glass vials, and the device measuring through the wall of the vials. All concentrations are quoted in volume agent/total volume percentages. Concentrations should be regarded as approximate.

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[1] B.A. Eckenrode, et.al, Foren. Sci. Comm. **3** (4), (2001); S.D. Harvey, et. al., Foren. Sci. Int. **125**, 12-21 (2002); D. Moore, Rev. Scientific Instruments **75**, (8), (2004).

Preliminary investigations of trace agent detection (HD and HN1) using surface enhanced Raman spectroscopy were also conducted.

2. DESCRIPTION OF THE TESTED HANDHELD INSTRUMENT

2.1 Principles of the Technology.

All molecules perpetually rotate, move, and contort in a complex manner at temperatures above absolute zero. Vibrational spectroscopy probes these contortions (or vibrations) of a sample to determine the chemical functional groups present. Two common types of vibrational spectroscopy are infrared (IR) absorption/reflectance and Raman. Both rely on illumination of the sample with optical radiation to probe the molecular vibrations.

In IR spectroscopy, the sample is illuminated with a broad spectrum of light in the mid-infrared region and the transmission or reflection is recorded as a function of the frequency of the incident light. When the frequency of incident light equals the frequency of a specific molecular vibration, the sample tends to absorb some of the light. A material "fingerprint" results from recording the amount of light absorbed as a function of the wavelength (or frequency).

In Raman spectroscopy, the sample is illuminated with monochromatic laser light and the scattered light is detected as a function of wavelength. The scattered light results from both elastic collisions (Raleigh scatter) of the photons with the sample's molecules as well as inelastic collisions (Raman scatter) which result in a drop in frequency of the inelastically scattered light. The inelastic collisions impart energy from the incident light to the modes of vibration of the molecules. A material "fingerprint" results from recording the intensity of the scattered light as a function of the energy difference between the laser and Raman scattered light.

Both Raman and IR spectroscopy create fingerprints for unique molecular identification of a sample; however, there are differences in the underlying physics; hence, each carries somewhat different, but complementary analytical information. It is coarsely estimated that for first responder field applications, approximately 70% of those materials of interest are both Raman and IR active. The level of uniqueness of Raman and IR molecular fingerprints is often similar for both IR and Raman, so both technologies hold promise for field-based materials characterization.

2.2 Instrument Hardware Characteristics.

Ahura's FirstDefender Product is a rugged handheld chemical identification unit designed for point-of-use applications. A photograph of the FirstDefender is shown in Figure 1. This product allows the identification of toxic industrial chemicals (TICs), narcotics, contraband, chemical weapons, and white powders using the principles of Raman spectroscopy. It is enclosed in a lightweight, rugged, and weather/chemical resistant package, weighs approximately 4 lbs and measures approximately 12" x 6" x 3". The unit is designed to operate

over a temperature range of -20 to +40 °C in dry (desert) and wet (tropical) environments. The product and its subsystems are individually verified to meet military and commercial environmental standards for water sealing, mechanical shock, mechanical vibration, and thermal shock. For details of compliance testing see Appendix B.

The FirstDefender product shown in Figure 1 has 3 modes of use. Two of the modes are "point-and-shoot" and the third is an in-vial measurement. The first mode of use is to place the targeting cone (shown at the top of the picture) onto the sample or container to be tested. In this mode, a metal cone contains the laser beam and keeps the needed focal distance to the sample. A second mode of use is to remove the laser cone and targeting foot to avoid coming in direct contact with the sample to be tested. In this mode the unit is ~1.5 cm above the sample, thus limiting potential contamination and user exposure. The third mode is a direct vial measurement. A hatch is present above the screen and beneath the logo marked area. When lifted, a hole is present for inserting a standard 4 mL test vial. The vial is positioned to allow measurements of both powders and liquids. The vials can then be saved for evidence collection or a confirmatory laboratory test.

The FirstDefender handheld contains a source laser, an optical probe for directing light to the sample and collecting the Raman scatter, and a spectrometer for analysis of the Raman spectrum. The optical subsystems are manufactured using Ahura's proprietary "optical engine" technology. This technology allows for the integration of tens of micro optical elements into a single compact (~1" square) hermetically sealed package. Each optical engine is produced in a controlled clean-room environment and each process is designed to be robust and reliable with mean times to failure beyond 10,000 hr (for active devices). Optical specifications of the resulting FirstDefender handheld are given in Table 1.

Table 1. FirstDefender Optical Specifications

Parameter	**Specification**
Monochrometer Spectral Range	781 nm-1014 nm
Raman Spectrum Range	250 cm^{-1} to 2875 cm^{-1}
Spectral Resolution	7 to 10 cm^{-1} (FWHM) across range
Laser (excitation wavelength)	785 nm +/- 0.5 nm (<2 cm^{-1} line width)
Laser Output	Settable, 30 mW, 100 mW, 300 mW
Rayleigh Rejection Filters	OD 7
Detector	Silicon CCD 2048 Pixels; TEC Cooled
Detection Mode	Direct Dispersive
Dispersion Mode	Single Pass Spectrometer (1200 groove/mm Blazed @ 900 nm)
Collection Optics	NA= 0.3

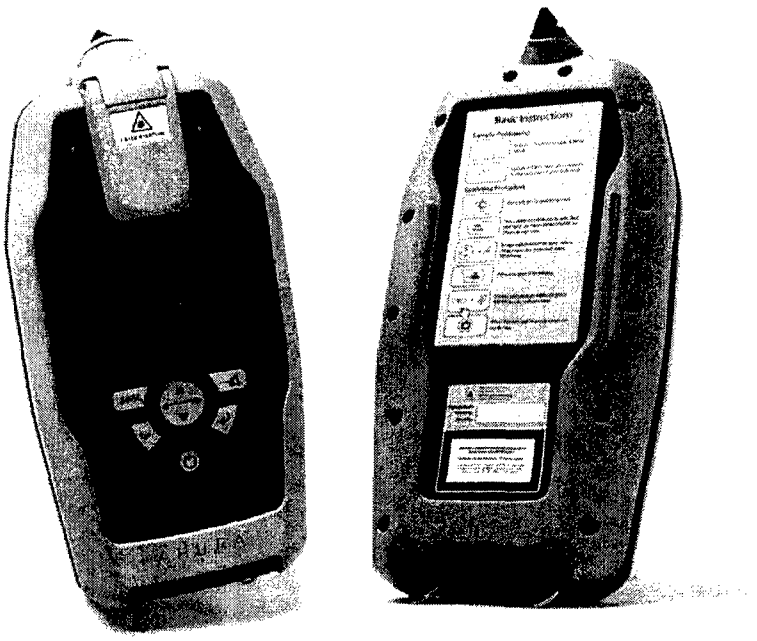

Figure 1. Rugged FirstDefender Raman-Based Handheld

2.3 Instrument Embedded Software.

The FirstDefender relies on embedded custom decision support software to compare the measured data to library records of known materials. The use of custom software is necessary for two reasons. First, no commercially available package is available for the limited resources of the onboard PXA255 400 MHz based single board computer. Secondly, commercial packages do not apply rigorous evidence-based match criteria, or provide automated formal mixture analysis.

The course architecture of the Ahura decision support software shown in Figure 2. Four distinct modules are integrated: Belief Engine, Data Engine, Mixture Engine and the Decision Engine. These modules have the following individual responsibilities.

Belief Engine™:	encode prior information available to the user
Data Engine™:	acquire data such that enough Raman information is available to make informed decisions; probabilistically assess the consistency of the acquired data with library records.
Mixture Engine™:	if the measured Raman data is not probabilistically consistent with any library record, propose mixtures of library records that explain the measured data.
Decision Engine™:	integrate information from the Belief Engine, Data Engine and Mixture Engine for probabilistic decision support.

As noted, the data engine drives data acquisition. The FirstDefender has two general modes of data acquisition: library mode, and normal measurement mode. In library mode the data engine collects data to a pre-specified level of high Raman fidelity. This is an important function, as low-quality library spectra severely limit the resolving power of the decision support software. In normal measurement mode—the mode employed for routine field testing—the data engine automatically chooses settings such that data is collected to a level of fidelity that resolves the vast majority of field samples, but minimizes the time required to execute a measurement. Normal measurement mode operation is therefore akin to the auto-exposure setting on most photographic cameras. Non-auto settings are available should an advanced user elect to override the system settings.

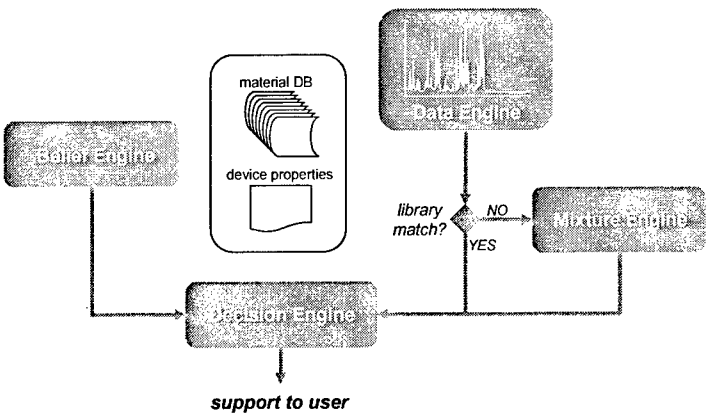

Figure 2. Architecture of the Embedded Decision Support Software in FirstDefender

Following the data collection, the data engine rules out library records that are probabilistically inconsistent with the measured data. If any library records remain that have not been ruled out, they are forwarded directly to the decision engine, which presents the user with information like the following:

1 plausible match found:

polystyrene **>99.9%**

INFO: The measured data is fully consistent with measurements of polystyrene.

The FirstDefender software does not report values akin to correlation or similar 'Hit Quality Indices'. In processing unseen to the user, it rules out library records if they are spectroscopically inconsistent with the measurement data. For those library records that cannot be ruled out, it reports posterior probabilities: the probability, based on the data, that the measured material is library Material A versus B, etc. In the case above all library records except polystyrene have been ruled out. Consequently, the probability that the sampled material is polystyrene is extremely high. The probability that it could be a different library material is

therefore extremely small (<<0.1%). This behavior is more evident in the next example, where multiple library records are consistent with the measured data:

2 plausible matches found. Sample could be

HN1 (nitrogen mustard) P=82.6%
or
HN3 (nitrogen mustard) P=17.3%

INFO: The measured data is consistent with only the above library records. The probabilities indicate how much the measured data favors one record versus another.

The decision support software has decided that BOTH of these materials are statistically consistent with the measurement data (*i.e.*, could not be ruled out). The probabilities are directly quantifying how much the evidence favors HN1 over HN3. (in this case the data suggests that HN1 is about 4 times more likely than HN3). Alternatively one could say that with probability 99.9% the material is either HN1 or HN3. In some circumstances the evidence will very strongly favor one of the reported matches (e.g., 94% v. 6%), while in other circumstances the evidence is less emphatic (*e.g.*, 52% versus 48%, or 40% versus 32% versus 28%).

If none of the library records are consistent with the data, an explanatory statement is issued to the user similar to "*NO PLAUSIBLE LIBRARY MATCH FOUND*" and the Mixture Engine module subsequently attempts to resolve the measured data using mixtures of library records. Library spectra of mixtures are not required. Candidate mixture models are generated by an optimization procedure, and are solved formally rather through user-directed sequential subtraction. If a mixture of library records is found that explains a significant portion of the measured Raman data, the user will be presented with a screen similar to the following:

Mixture found:

Constituents	recovery
VX (nerve agent)	**64.7%**
Cluster	**34.9%**
↳Diesel #2	
↳JP8 (jet fuel)	
total	*99.6%*

INFO: The measured data can not be adequately described by a single library record. A mixture of the above constituents is able to account for a large amount of the measured Raman data. The % values reported are NOT concentrations—they are the amount of Raman data that can be described by each constituent.

Note that one of the constituents is called "Cluster", and has two members: Diesel #2 and JP8 (jet fuel). The Mixture Engine 'clusters' library records that are very similar in Raman spectral response to speed and condition computational aspects of the mixture solution. If the proposed solution contains a cluster, as it does in the above example, it implies that a statistically equivalent solution could be obtained by using either of the members of the cluster. It is also important to note that the percentages reported for mixtures do not correspond to concentrations. They represent the amount of measured Raman data that is accounted for (recovered) by the inclusion of a particular constituent in the mixture solution. For the example above, the 64.7% of the Raman activity of the sample can be attributed to VX, and 34.9% can be attributed to one of Diesel #2 or JP8. The Mixture Engine has the capacity to solve for up to 6 individual components to, although the success at this level of complexity will vary based on the concentrations and identities of the components involved.

The overall decision tree for the decision support software embedded on the FirstDefender is summarized in Figure 3.

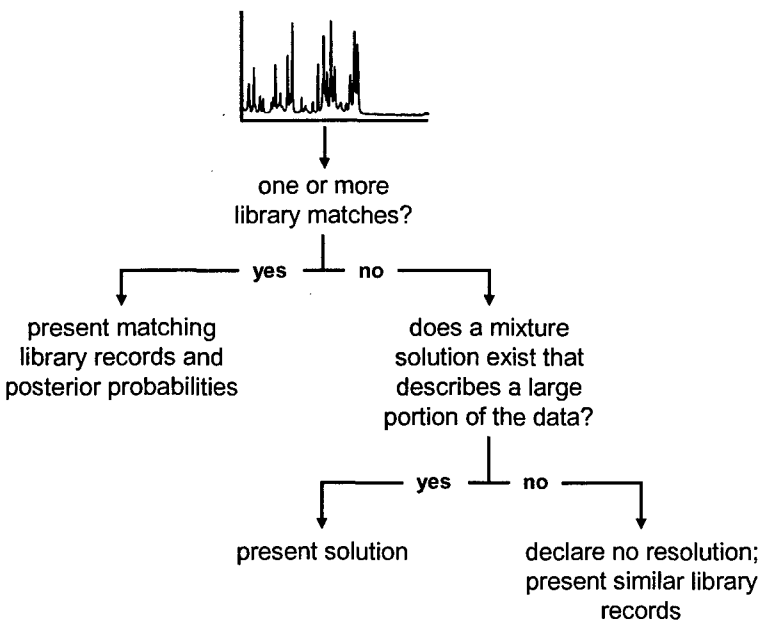

Figure 3. Decision Tree for the Embedded Decision Support Software in FirstDefender

3. EXPERIMENTAL PROCEDURES

3.1 Neat Agent Testing.

Pure agent testing was conducted on the FirstDefender handheld unit (Serial # FDEC0401). Three steps were performed: (1) Add-to-library, (2) Verification scan using the vial holder, (3) Verification scan using the point-and-shoot mode.

3.1.1 Add-to-Library.

Approximately 0.5 mL of agent was dispensed into a standard 4 ml vial (VWR Part# 66009-981). A list of the exact quantities, agent purities, and lot information is given in . The quantity was selected to allow convenient interrogation of the sample within the vial holder; smaller quantities can be used. The scan mode was then set to add-to-library with the highest quality setting possible for the available time. The majority of agents were measured using HIGH quality with total integration times of ~ 8 min. Following scan completion, the add-to-library menu function was selected and the collected spectrum was added to the on-board chemical library using a user entered name.

Table 2. Agent Reference Information

Agent	Purity	Amount Used (mL)
HD	97.3%	0.43
HN1	97.8%	0.47
HN3	99.8%	0.54
L	95.9%	0.48
VX	96.2%	0.38
GB	98.7%	0.63
GA	98.5%	0.34
GF	96.6%	0.48
GD	98.8%	0.42

3.1.2 Verification Scan (Using Vial Holder).

Two verification scans were performed following each addition of agent spectrum to the library. The first verification scan was performed in the vial holder. Following library building, the vial was removed from the holder and purposely rotated and reinserted into the holder. The scan mode was then set to AUTO mode and a scan initiated.
The results of the verification scan were then displayed.

3.1.3 Verification Scan (Using Point-and-Shoot).

A second verification scan was performed using the point-and-shoot mode. The nose of the unit was placed against the glass vial containing the agent. The unit was held by hand in position. The nose cone was set on the handheld to be depressed fully to allow the focus of the laser to be inside the glass vial wall. The scan mode was set to AUTO mode and a scan initiated. The results of the verification scan were then displayed.

3.2 Agent and Interferent Testing.

Following the addition of the pure agents to the signature library, the spectra from three spectra of potential interfering substances were added to the library using a similar approach as for the neat agents. The interferents measured include: JP8 Jet Fuel, Floor Wax, and Aqueous Film Forming Foam (AFFF). Windex was used as an interferent in testing, but was not separately added to the library given that 2-propanol (the dominant component of Windex) was already in the library. Mixture samples were prepared by mixing the neat agent with the interferences to achieve desired concentrations. Agent concentrations ranging from 66% to 1.25% (v/v) were studied. Each prepared sample was dispensed into a sealed glass vial, and measured in the FirstDefender vial holder using the AUTO scan mode.

3.3 Trace Agent Investigation.

When a molecule is adsorbed on a nanometer-scale roughed silver or gold surface, or is mixed with gold or silver nano-particle sol-gel, the Raman scattering cross section can be enhanced tremendously, a phenomenon called surface enhanced Raman scattering (SERS).[2] The dominant enhancement mechanism in this process is the nanometer scale enhanced electromagnetic field near the metallic surface. The bulk enhancement factor may reach 106 for some molecules, enabling trace detection (ppm to ppb) of many species. Scientific interest in surface enhanced Raman spectroscopy continues to increase, so in addition to the aforementioned FirstDefender product testing, experiments were performed to investigate the feasibility of extending the FirstDefender product platform to trace detection using SERS. These experiments were conducted by mixing low-level concentrations of agent with Ahura's proprietary sol-gel matrix

3.4 Operating Performance Verification.

Environmental testing, as outlined in Appendix B was performed on the Ahura FirstDefender Unit at MET Laboratories in Baltimore, MD. A brief verification of low temperature storage, low temperature operation, and battery life was also conducted at ECBC.

3.4.1 Low-Temperature Testing.

FirstDefender Unit (Serial # FDEC1602) was placed in an environmental chamber cooled to -20 °C at ambient humidity. The unit soaked in this environment for >12 hr in a sleep state with the battery inserted. The unit was then woken from sleep in the chamber and observed. The unit was then immediately brought into a warm and humid laboratory environment and a measurement of polystyrene was performed in the vial holder.

[2] K. Kneipp, H. Kneipp, I. Itzkan, R. R. Dasari, and M. S. Feld, "Ultrasensitive Chemical Analysis by Raman Spectroscopy", Chem. Rev. 99, 2957-2975 (1999); Farquharson, S.; Maksymiuk, P.; Ong, K.; Christesen, S. "Chemical agent identification by surface-enhanced Raman spectroscopy", SPIE, 4577, 166-173 (2001).

3.4.2 Battery Life.

All testing conducted at ECBC was done under battery power. An external docking station was used to recharge spent Lithium ion batteries as needed. The battery life was tracked by monitoring the start time of fresh battery insertion and the shutdown time due to a low battery. The unit was operated continuously at a temperature of ~28 °C (without auto or manual sleep/wake operations) within a chemical fume hood.

4. RESULTS AND DISCUSSION

4.1 Overview.

The device as tested had a version of the decision support software that executed the probabilistic library match analysis, but the software for automatic mixture analysis (the Mixture Engine) was not embedded at the time. Therefore the unit executed pure-component analysis in real-time, and the spectroscopic data was taken back to Ahura so that the data could be used offline with mixture analysis software on a standalone PC. At the time of FirstDefender release the automatic mixture analysis software will be embedded on the unit.

Some examples of Raman spectra of pure agents and mixtures that were collected during the course of testing are shown in Figure 4. The top pane of Figure 4 shows the Raman spectra of pure GA and pure VX that were added to the spectral library on the unit. The bottom pane shows the Raman spectra resulting from a measurement of 25% GA in floor wax, and 25% VX in JP8 jet fuel collected in AUTO mode. AUTO measurement times were typically 1 to 5 sec, although for some samples up to 20 sec was required to achieve the target quality.

One of two key findings on the first day of data acquisition was that GF (cyclosarin) exhibited substantial fluorescence, so much so that field detection of this agent will be very difficult to achieve with reasonable measurement times. It was therefore not included in the library, and mixtures of GF and interferents were not examined in subsequent days.

The other key finding was that the two nitrogen mustards (HN1 and HN3) were moderately fluorescent, although characteristic Raman scatter was observable with reasonable measurement times. These were individually added to the library, although the two agents will be very difficult to discern from one another with short measurement times. As noted in Section A.4 the mixture analysis software automatically clusters library entries that are extremely difficult to individually resolve in mixtures. The individual case results reflect this behavior—when strong evidence of HN1 or HN3 was found in a mixture, the analysis software presents both as plausible constituents. Given the spectral and molecular structure similarity of HN1 and HN3, we elected to investigate only one of the entities (HN3) in agent and interferent mixtures, under the assumption that the detection characteristics for HN1 would be similar.

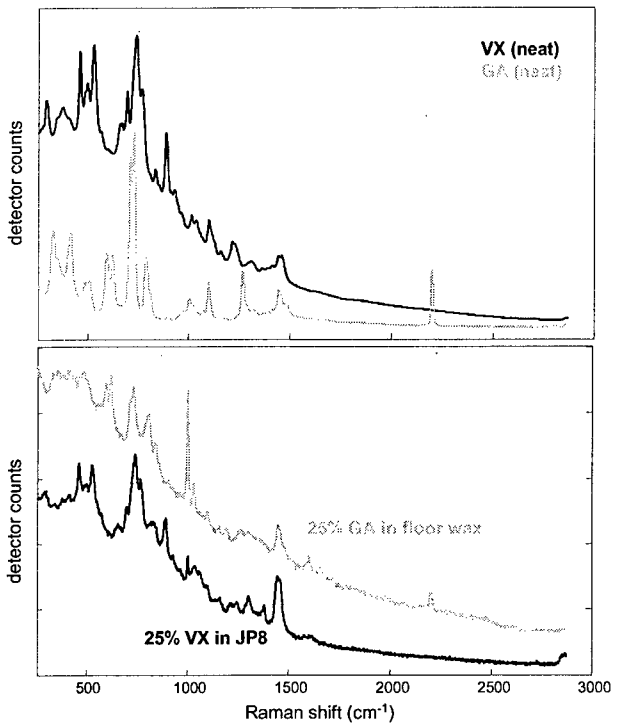

Figure 4. Examples of Spectral Data Collected in the Course of FirstDefender Testing. Top: spectra of neat VX and GA that were added to the library on the handheld device. Bottom: spectra acquired in auto-exposure mode that were used for device performance testing.

4.2 Neat Agent Testing.

Library spectra of the pure agents and interferents were acquired on the first day of experimentation. Immediately following the library measurement and addition, confirmation measurements were taken of the agent in auto-exposure mode. Some measurements of neat agents were also taken on subsequent days to verify system performance. In all 12 (non-library) measurements of the neat agents were taken with the agent in glass vials in the FirstDefender vial holder, and 10 free-space measurements of the neat agents were taken.

For 21 of the 22 neat-agent AUTO measurements FirstDefender reported true-positive detection of the appropriate agent. In the one exception (a free-space measurement of HN1), it was noted that aiming alignment was off and the agent itself was not being interrogated by the device. In this case the analysis algorithms appropriately reported that no plausible match could be found.

No false positives were observed for the 22 neat-agent measurements, that is, the decision support software reported only one plausible match for each measurement; however, measurements of HN1 and HN3 were an exception. As noted above, these two agents are difficult to discern from one another with short measurement times, and in most instances the analysis algorithms reported that both HN1 and HN3 were plausible matches when either neat HN1 or neat HN3 was being measured.

A concise summary of the neat-agent case results are given in Table 3, and more detail is available in the detailed case reports in the Appendix C.

Table 3. Pure Agent Measurements. Each measurement is enumerated as date/'session#/scan#'

AGENTS	VIAL HOLDER	FREE SPACE
HD	Apr18/001/005: 1 match HD (distilled mustard, Blister agent) Prob >99.9%	Apr18/001/006: 1 match HD (distilled mustard, Blister agent) Prob >99.9%
HN1 †	Apr18/001/009: 1 match HN1 (nitrogen mustard) Prob >99.9% Apr18/002/010: 2 plausible matches (total Prob 99.8%) HN1 (nitrogen mustard) Prob 89.5% HN3 (nitrogen mustard) Prob 10.3%	Apr18/001/010 NO PLAUSIBLE MATCH FOUND {sample misalignment, see § at bottom of table} Apr18/001/011: 1 match HN1 (nitrogen mustard) Prob >99.9%
HN3	Apr18/001/014: 2 plausible matches (total Prob >99.9%) HN1 (nitrogen mustard) Prob 66.0% HN3 (nitrogen mustard) Prob 34.0%	Apr18/001/015: 2 plausible matches (total Prob >99.9%) HN1 (nitrogen mustard) Prob 61.5% HN3 (nitrogen mustard) Prob 38.5%
VX	Apr18/001/017: 1 match VX (Nerve agent) Prob >99.9% Apr19/002/015: 1 match VX (Nerve agent) Prob >99.9% Apr21/001/011: 1 match VX (Nerve agent) Prob >99.9%	Apr18/001/018: 1 match VX (Nerve agent) Prob >99.9%
GA	Apr18/001/020: 1 match GA (tabun nerve agent) Prob >99.9%	Apr18/001/021: 1 match GA (tabun nerve agent) Prob >99.9%
GB	Apr18/001/023: 1 match GB (sarin nerve agent) Prob >99.9%	Apr18/001/024: 1 match GB (sarin nerve agent) Prob >99.9%
GD	Apr18/001/026: 1 match GD (soman nerve agent) Prob >99.9%	Apr18/001/027: 1 match GD (soman nerve agent) Prob >99.9%
L	Apr18/002/003: 1 match L (lewisite blister agent) Prob >99.9% Apr 18/002/004: 1 match L (lewisite blister agent) Prob >99.9%	Apr18/002/005: 1 match L (lewisite blister agent) Prob >99.9% Apr21/001/Scan012: 1 match L (lewisite blister agent) Prob >99.9

† The measurements denoted Apr18/001/009-011 were taken before HN3 was added the spectral library, while the measurement denoted Apr18/002/010 was taken after the addition of HN3 to the library.

§ Aiming alignment was off such that the agent was not actually being sampled.

4.3 Mixture/Diluted Agent Testing.

Testing of mixtures of 7 CW agents[3] with 4 different interferents at various concentrations occurred over the course of three days, totaling 66 different cases. In 22 of 66 cases, the Raman signal from the interferent was nearly or completely unobservable, and the analysis algorithms were able to positively confirm the presence of the agent by pure analysis only. In the remaining cases (44 of 66), the data engine could not find library records fully consistent with the measured data—suggestive of a mixture, or chemical species not represented in the library—and the sample measurement was analyzed for mixtures of substances. The presence of agent was correctly suggested in 35 of these 44 cases by mixture analysis. In total, then, CW agents were positively detected in 57 of 66 cases, summarized in Table 4.

Table 4. Positive Detection Case Summary

HD	positive detection in all cases
HN3	positive detection in all cases
VX	positive detection in Windex at and above 25% VX, positive detection in JP8 jet fuel in all cases, positive detection in AFFF at 50% VX
GA	positive detection in Windex at and above 12.5% GA; positive detection in JP8 jet fuel in all cases; positive detection in AFFF in all cases; positive detection in floor wax at and above 25% GA
GB	positive detection in all cases
GD	positive detection in all cases
L	positive detection in Windex in all cases; positive detection in JP8 jet fuel at 50% L; positive detection in AFFF in all cases

The 9 cases in which the agent was not detected are summarized in Table 5.

Table 5. Failed Detection Case Summary

VX	failure to detect in Windex at concentrations at and below 10% (4 cases); failure to detect in AFFF at 25% (1 case)
GA	failure to detect in Windex at concentrations at and below 6.25% (2 cases)
GA	failure to detect in floor wax at 12.5% (v/v) (1case)
L	failure to detect in JP8 jet fuel at 25% (1 case)

[3] The reader is reminded that HN1 was not evaluated in agent + interferent mixtures. Due to the substantial spectral and molecular similarity between HN1 and HN3, it was thought to be more important to evaluate a wider range of agent + interferent mixtures in the allotted time. While we expect the results for HN1 to be very similar to the results for HN3, this is, as of yet, unconfirmed.

A quick summary view of all cases is provided in Table 6.

Table 6. Mixture Measurement Result Summary. Boxes that are grayed out correspond to solutions that were not run. Results for each case are summarized using the following legend:

- ✓ | NA — data engine was able to confirm a pure match for the agent; mixture analysis was therefore not applicable
- × | ✓ — data engine could not confirm a pure match to any library entry; mixture analysis resolved the mixture and detected the agent
- × | × — algorithm could not confirm a pure match to any library entry; mixture analysis did not find a satisfactory solution, or did not detect the agent in that solution

AGENTS	v/v %	Windex	JP8 jet fuel	AFFF	floor wax
HD	50%		✓ | NA	✓ | NA	
	25%		× | ✓	✓ | NA ✓ | NA	
HN1	*				
HN3	50%	✓ | NA	✓ | NA	✓ | NA	
	25%	✓ | NA	× | ✓	✓ | NA	
VX	50%	× | ✓ ✓ | NA	✓ | NA × | ✓	× | ✓	
	25%	× | ✓ × | ✓ × | ✓	× | ✓ × | ✓	× | ×	
	10%	× | ×			
	5%	× | ×			
	2.5%	× | ×			
	1.25%	× | ×			
GA	50%	× | ✓	✓ | NA	✓ | NA	× | ✓
	25%	× | ✓	✓ | NA	× | ✓	× | ✓
	12.5%	× | ✓	✓ | NA	× | ✓	× | ×
	6.25%	× | ×		× | ✓	
	3.125%	× | ×			
GB	50%	✓ | NA	✓ | NA	✓ | NA	
	25%	✓ | NA	× | ✓ × | ✓ × | ✓	× | ✓	
	12.5%	× | ✓			
GD	50%	× | ✓	✓ | NA	× | ✓	
	25%	× | ✓		× | ✓	
	12.5%	× | ✓		× | ✓	
L	66%			✓ | NA	
	50%	× | ✓	× | ✓ × | ✓ × | ✓	✓ | NA	
	25%	× | ✓	× | ×	× | ✓	

* HN1 and HN3 were substantively similar in properties and Raman cross section, so we elected to only investigate the behavior of HN3 and assume that the behavior for HN1 would be highly similar.

In many cases requiring mixture analysis both the agent AND interferent were simultaneously identified. For example, the measurement of 25% GA in butchers floor wax (Apr20/001/006) resulted in the following mixture analysis report:

Constituents	recovery
Cluster	90.28%
↳Polystyrene	
↳butchers floor wax	
GA (tabun nerve agent)	7.22%
TOTAL	97.50%

The measurement of 25% VX in JP8 jet fuel (Apr21/001/020) resulted in the following:

Constituents	recovery
VX (nerve agent)	66.74%
Cluster	34.98%
↳Diesel #2	
↳JP8 jet fuel	
TOTAL	101.72%

Full resolution of mixtures was not always as successful. For example a case of 12.5% GA in Windex (Apr19/003/015) resulted in the following mixture solution which a large proportion of the measured data remains unexplained, even though GA and 2 propanol (a component of Windex) are likely the dominant species in the mixture. In this and many similar cases, by interpretation of the measured Raman spectrum it appears that an interaction between the agent and diluent caused a departure from linear additivity, meaning that the spectrum of the mixture was not approximately the spectrum of the two constituents, which detracts from the decision support software's ability to approximate the mixture with combinations of library materials. The likely mechanism of this departure is aggressive hydrogen bonding for some aqueous mixtures, an effect that could be mitigated to some degree if aqueous solutions of agents (agents in pure water) were also added to the spectral library, although as evidenced by the results in Table 6, this course of action in not necessary for positive detection.

Constituents	recovery
GA (tabun nerve agent)	44.66%
2-propanol	18.61%
TOTAL	63.26%

Search Precision.

Although true positive rate (positive detection when agent is present) is a critical parameter for deployable chemical detectors, false-positive attributes are also important. The above testing does not constitute a comprehensive evaluation of false-positive rates for CW agents; however, it does allow for an assessment of a related measure relevant for chemical identification systems: search imprecision. For field-portable chemical identifiers like the FirstDefender the material search could return no matching library records, one matching record, or multiple records. Clearly if the identifier returned a large number of matching records for every analysis it is more likely to present the correct compound in the list, but for the field user a short list of materials is more valuable than a long list.

To quantify this behavior we define search imprecision as the number of incorrect positive matches that are returned by the search software. A search that only returns the correct library record (or records if it is a mixture) has imprecision 0. When two library records are returned but only one of them is correct, the imprecision is 1, etc. The tabulated results for all measurements conducted in the course of this testing are given in Table 7. Note that for one measurement—25% L in JP8 jet fuel—the decision support software did not report a library match, or come to a mixture resolution. While this case is logged as a failed detection condition in Table 5, a null result to the user has no associated imprecision. Similarly, a neat agent of test of HN1 also resulted in a null report. The remaining 86 cases are reported below. Cumulative percentages are given in the last column, indicating the percent of cases with imprecision equal to or better than the corresponding row imprecision.

Table 7. Summary of Search Precision over All Cases

Imprecision	Cases	Cumulative
0	58	67.4%
1	21 (9 HN1+HN3 cases)	91.8%
2	3	95.3%
3	3	98.8%
4	1	100%
Total	86	

One can not take the above cumulative percentages as 'population' estimates, since the presence of components like HN1/HN3 skews the results, but for the testing as presented, in 67.4% of cases zero non-relevant library records were returned in the search, and in 91.8% of cases one or zero non-relevant library records were returned by the FirstDefender decision support software. A large fraction (42.8%) of the 21 cases with imprecision 1 were due to the spectral ambiguity between HN1 and HN3.

4.4 Trace Agent Investigation.

Surface enhanced Raman spectroscopy (SERS) was examined using several agents and concentrations. The surface enhanced Raman spectrum of distilled mustard (HD) solution (after correction for the pure sol-gel spectrum) is shown in Figure 5. The sample was prepared using the following procedures: 1μL of neat HD was mixed with 1 μL H2O. The resulting solution was diluted with 2 mL H2O. 20 μL of the diluted solution was mixed with 180 μL H2O and 200 μL silver sol-gel solution. 400 μL NaCl was finally added to activate the solution. The concentration of HD agent in the final solution was therefore approximately 12.5 ppM (v/v).

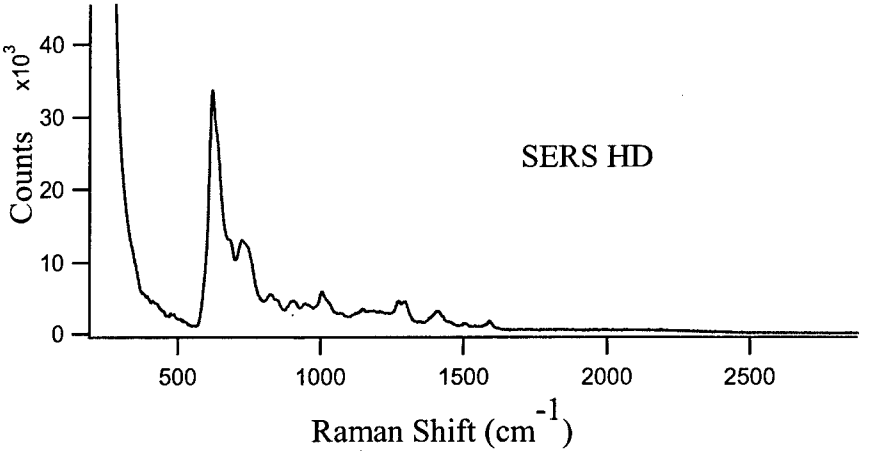

Figure 5. SERS Spectrum of 12.5 ppM HD Corrected for the Spectrum of the Sol-Gel Matrix

A SERS spectrum of HN1 was obtained using a similar procedure to a final concentration of approximately 1.25 ppthousand (v/v). The resulting spectrum after sol-gel matrix correction is shown in Figure 6.

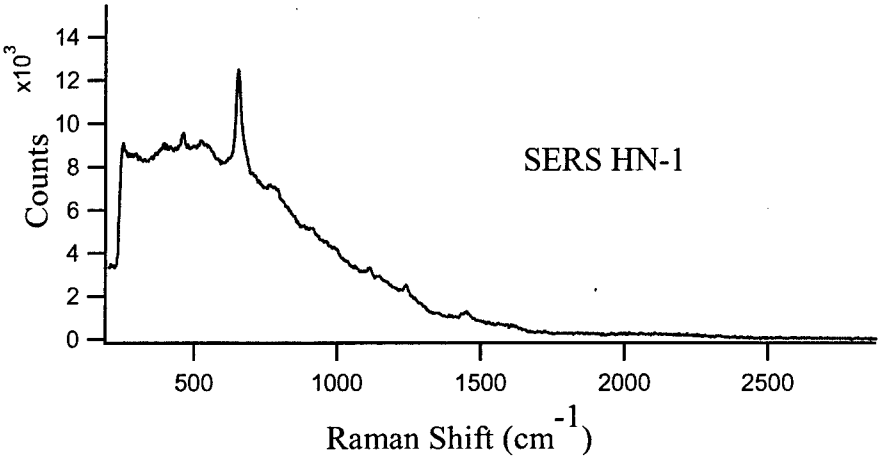

Figure 6. SERS Spectrum of HN1 at a Concentration of 1.25 ppthousand (v/v) Corrected for the Spectrum of the Sol-Gel Matrix

Although considerable work remains to demonstrate the commercially reliable performance of this FirstDefender SERS platform, the results obtained in these early investigations are encouraging for trace detection of CW agents.

4.5 Operational Testing.

4.5.1 Battery Life.

The system employed in routine testing for neat agents was timed for battery life. A fresh battery was inserted and the unit was turned on at 8:10 am on the morning of Apr 18th. The unit was used continuously (except for a 1 ½ hr suspended state over lunch) until 2:30 pm at which point the battery was exhausted, totaling about 5 hr of continuous operation.

4.5.2 Low-Temperature Testing.

As discussed in detail in Section B.4, a FirstDefender unit was subjected to an environmental chamber with uncontrolled humidity for >12 hr While still in the chamber, the unit was cleared of frost that had accumulated on the device, and wakened from sleep to verify that the battery remained functional. It was later removed from the chamber into a warm and humid laboratory environment where a measurement of polystyrene was performed in AUTO mode with the sample in the vial holder. The FirstDefender decision support software indicated a positive match only for polystyrene (Prob >99.9%).

5. CONCLUSION

The chemical weapons (CW) detection capability of Ahura Corporation's FirstDefender handheld Raman chemical identification system was incorporated and confirmed through testing of both neat CW agents and a broad range of agent + interferent mixtures through the walls of sealed glass containers. The system correctly identified the CW agent under consideration in 78 of 88 cases tested. Twenty two of these cases were neat agents, and the remaining cases were mixtures of agent and one of JP8 jet fuel, aqueous film forming foam, Windex, and floor wax at concentration levels from 50% to 1.125% agent by volume. The failures in agent detection were largely at agent concentrations at or below 10% in Windex. In spite of the system's inability to reliably differentiate between the presence of HN1 and HN3 in routine field measurements due to their highly similar Raman spectrum, it did identify correctly the potential presence of nitrogen mustard either as HN1 or HN3.

In summary, given the range of operating characteristics in which this device can successfully operate, the self-contained non-contact/non-destructive nature of the system, and the CW detection performance tested; the FirstDefender can be suitable for (non-trace) field detection and identification of liquid that may contain CW agents.

APPENDIX A
AHURA'S BACKGROUND

Ahura Corporation was founded as a Delaware corporation in March of 2002 around a team of scientists and engineers to develop innovative cost-effective high-performance optical solutions for a broad array of markets. Ahura is a small business concern that has raised more than $20M from top tier venture capital firms including ComVentures, ARCH Venture Partners, and Castile Ventures. The Company is focused on developing, manufacturing, and selling Raman based products based on proprietary optical engines and software platforms.

Ahura Corporation is comprised of an innovative team of scientists and engineers in a vertically integrated facility, bringing a cross-disciplinary approach to the challenges facing our society. Ahura is located in a 30,000 square foot facility in Wilmington, MA. The majority of this space is dedicated to engineering development and manufacturing including: an MOCVD semiconductor laser growth facility, chip fabrication and thin-film development, ultra-compact optical package development lab and production line, electronic system design and test capability, full electrical and optical test infrastructure, reliability and failure analysis room, and highly equipped machine shop. In addition to these facilities, the company has software design tools for lasers, thin-film passive optics, packaging, electronic circuit design, and software algorithm development. The remaining space is used for inventory, shipping and receiving, and office space.

Blank

APPENDIX B
COMPLIANCE TESTING

The MIL-STD-810F standards met by this product are listed in Table B.1. Transit shock testing is currently in progress. Testing to the military standards was conducted by the company through a third party laboratory; MET Laboratories in Baltimore, MD. A letter of compliance to these standards is given in Figure B.1 for reference. A detailed test report is available from MET Laboratories.

Table B.1 – Qualification Tests Passed for the FirstDefender Handheld

Qualification Test	Detail	Condition
Mechanical Shock	MIL-STD-810F (516.5) Procedure I	Ground Equipment, 40g, 11ms, saw tooth
Vibration	MIL-STD-810F (514.5) Procedure I (Composite Wheeled Vehicle)	1 hr / axis, Category 20 - Composite Wheeled Vibration Exposure
Humidity	MIL-STD-810F (507.4)	5X (48 hr) 60C & 95% RH
Sand & Dust	MIL-STD-810F (510.4) Procedure I	Blowing Dust
Water Immersion	MIL-STD-810F (512.4)	1 meter for 30 min
Thermal Shock	MIL-STD-810F (503.4) Procedure I	<1 min Transition -30 to +60C, 1 day
Low Temp. (Operation)	MIL-STD-810F (502.4) Procedure II	-20C 1 day exposure following stabilization (Restrained Glass)
High Temp. (Storage)	MIL-STD-810F (501.4) Procedure I	+60C 7 days exposure
Low Temp. (Storage)	MIL-STD-810F (502.4) Procedure I	-30C 1 day exposure

The FirstDefender has been designed to be compliant with commercial emissions, laser safety, and product safety regulations. A list is given below:

- SAFETY: The product is being designed to comply with UL-61010-1 and CSA C22.2 No. 61010-1 safety standards.

- LASER SAFETY: Complies with FDA CDRH 1040.1 & IEC60825

- EMISSIONS: FCC Part 15 Subpart B-Unintentional Radiators and ICES-003 Industry Canada Interference-Causing Equipment Standard-Digital Apparatus specifications. Specifically our unit has been tested to comply with 15.107 conducted emissions and 15.109 radiated emissions.

MET Laboratories, Inc.
914 W. Patapsco Ave. Baltimore MD 21230
410-354-3300. Fax: 410-354-3313. 800-638-6057 www.metlabs.com

June 7, 2005

Ahura Corporation
46 Jonspin Road
Wilmington, MA 01887

Dear Kevin Knopp,

Congratulations! It is our pleasure to inform Ahura Corporation that the First Defender Handheld Identification System (FD-2000), as will be defined in the MET Laboratories' Test Report ESL17000-MIL, has completed the following testing at MET Laboratories, Inc for *MIL-STD-810-F:*

Method 501.4 High Temperature

Procedure I - Storage (High Temp) – Complete and Compliant

Procedure II - Operation (High Temp) – Complete and Compliant

Method 502.4 Low Temperature

Procedure I - Storage (Low Temp) – Complete and Compliant

Procedure II - Operation (Low Temp) – Complete and Compliant

Method 503.4 Temperature Shock

Procedure I - Steady State – Complete and Compliant

Method 507.4 Humidity – Complete and Compliant

Method 510.4 Sand and Dust

Procedure I - Blowing Dust – Complete and Compliant

Method 512.4 Immersion

Procedure I – Immersion – Complete and Compliant

Method 514.5 Vibration

Category 20 - Ground Vehicles - Ground Mobile – Complete and Compliant

Method 516.4 Mechanical

Procedure I - Functional Shock – Complete and Compliant

Procedure IV – Transit Drop – Complete and Compliant

Method 516.5 Shock

Procedure I - Functional Shock – Complete and Compliant

For specific details regarding the extent of the testing and the configuration of the product tested, please consult the MET Laboratories' Detailed Test Report. Please contact me with any questions or comments.

Sincerely,

Todd Talbot

Todd Talbot
Manager, Environmental Simulation Laboratory

Figure B.1 - MET Laboratories Letter of MIL-STD-810F Compliance

APPENDIX C
INDIVIDUAL CASE REPORTS

The individual case reports are formatted as follows:

case file identification information technician observations truth condition	device results report: Pure component library search summary Mixture analysis summary (if necessary)

2005-04-18

SESSION 001

Cases 1,2 were HgAr spectrum and Acetonitrile/Toluene spectra respectively.

\\FDEC1602_ROOT\FDEC1602\20050418\History\Session001\raw003.spc

pure polystyrene	Session001; scan003; match=Polystyrene (>99.9%) 'LRD #' 'component' 'A0001' 'Polystyrene'

\\FDEC1602_ROOT\FDEC1602\20050418\History\Session001\raw004.spc

HD (distilled mustard)	Session001; scan004; match=NO PLAUSIBLE LIBRARY MATCH FOUND MATERIAL ADDED TO LIBRARY

\\FDEC1602_ROOT\FDEC1602\20050418\History\Session001\raw005.spc

HD (distilled mustard)	Session001; scan005; match=HD (distilled mustard) (>99.9%) 'LRD #' 'component' 'U001PI1' 'HD (distilled mustard)'

\\FDEC1602_ROOT\FDEC1602\20050418\History\Session001\raw006.spc

HD (distilled mustard)	Session001; scan006; match=HD (distilled mustard) (>99.9%) 'LRD #' 'component' 'U001PI1' 'HD (distilled mustard)'

FDEC1602_ROOT\FDEC1602\20050418\History\Session001\raw007.spc

HN1 (nitrogen mustard)	Session001; scan007; match = NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND

\\FDEC1602_ROOT\FDEC1602\20050418\History\Session001\raw008.spc

HN1 (nitrogen mustard)	Session001; scan008; match = NO PLAUSIBLE LIBRARY MATCH FOUND MATERIAL ADDED TO LIBRARY

\\FDEC1602_ROOT\FDEC1602\20050418\History\Session001\raw009.spc

HN1 (nitrogen mustard)	Session001; scan009; match=HN1 (nitrogen mustard) (>99.9%) 'LRD #' 'component' 'U03M4KS' 'HN1 (nitrogen mustard)'

\\FDEC1602_ROOT\FDEC1602\20050418\History\Session001\raw010.spc

HN1 (nitrogen mustard)	Session001; scan010; match = NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND

\\FDEC1602_ROOT\FDEC1602\20050418\History\Session001\raw011.spc

HN1 (nitrogen mustard)	Session001; scan011; match=HN1 (nitrogen mustard) (>99.9%) 'LRD #' 'component' 'U03M4KS' 'HN1 (nitrogen mustard)'

\\FDEC1602_ROOT\FDEC1602\20050418\History\Session001\raw012.spc

HN3 (nitrogen mustard)	Session001; scan012; match= NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND

\\FDEC1602_ROOT\FDEC1602\20050418\History\Session001\raw013.spc

HN3 (nitrogen mustard)	Session001; scan013; match= NO PLAUSIBLE LIBRARY MATCH FOUND MATERIAL ADDED TO LIBRARY

\\FDEC1602_ROOT\FDEC1602\20050418\History\Session001\raw014.spc	
HN3 (nitrogen mustard)	Session001; scan014; match= 2 PLAUSIBLE MATERIALS (total >99.9% posterior) 'LRD #' 'component' 'U005P45' 'HN3 (nitrogen mustard)' 'U03M4KS' 'HN1 (nitrogen mustard)'
\\FDEC1602_ROOT\FDEC1602\20050418\History\Session001\raw015.spc	
HN3 (nitrogen mustard)	Session001; scan015; match= 2 PLAUSIBLE MATERIALS (total >99.9% posterior) 'LRD #' 'component' 'U005P45' 'HN3 (nitrogen mustard)' 'U03M4KS' 'HN1 (nitrogen mustard)'
\\FDEC1602_ROOT\FDEC1602\20050418\History\Session001\raw016.spc	
VX (nerve agent)	Session001; scan016; match= NO PLAUSIBLE LIBRARY MATCH FOUND MATERIAL ADDED TO LIBRARY
\\FDEC1602_ROOT\FDEC1602\20050418\History\Session001\raw017.spc	
VX (nerve agent)	Session001; scan017; match=VX (nerve agent) (>99.9%) 'LRD #' 'component' 'U021XKJ' 'VX (nerve agent)'
\\FDEC1602_ROOT\FDEC1602\20050418\History\Session001\raw018.spc	
VX (nerve agent)	Session001; scan018; match=VX (nerve agent) (>99.9%) 'LRD #' 'component' 'U021XKJ' 'VX (nerve agent)'
\\FDEC1602_ROOT\FDEC1602\20050418\History\Session001\raw019.spc	
GA (tabun nerve agent)	Session001; scan019; match= NO PLAUSIBLE LIBRARY MATCH FOUND MATERIAL ADDED TO LIBRARY
\\FDEC1602_ROOT\FDEC1602\20050418\History\Session001\raw020.spc	
GA (tabun nerve agent)	Session001; scan020; match=GA (tabun nerve agent) (>99.9%) 'LRD #' 'component' 'U048DAT' 'GA (tabun nerve agent)'

\\FDEC1602_ROOT\FDEC1602\20050418\History\Session001\raw021.spc

GA (tabun nerve agent)	Session001; scan021; match=GA (tabun nerve agent) (>99.9%) 'LRD #' 'component' 'U048DAT' 'GA (tabun nerve agent)'

\\FDEC1602_ROOT\FDEC1602\20050418\History\Session001\raw022.spc

GB (sarin nerve agent)	Session001; scan022; match= NO PLAUSIBLE LIBRARY MATCH FOUND MATERIAL ADDED TO LIBRARY

\\FDEC1602_ROOT\FDEC1602\20050418\History\Session001\raw023.spc

GB (sarin nerve agent)	Session001; scan023; match=GB (sarin nerve agent) (>99.9%) 'LRD #' 'component' 'U03JO2U' 'GB (sarin nerve agent)'

\\FDEC1602_ROOT\FDEC1602\20050418\History\Session001\raw024.spc

GB (sarin nerve agent)	Session001; scan024; match=GB (sarin nerve agent) (>99.9%) 'LRD #' 'component' 'U03JO2U' 'GB (sarin nerve agent)'

\\FDEC1602_ROOT\FDEC1602\20050418\History\Session001\raw025.spc

GD (soman nerve agent)	Session001; scan025; match = NO PLAUSIBLE LIBRARY MATCH FOUND MATERIAL ADDED TO LIBRARY

\\FDEC1602_ROOT\FDEC1602\20050418\History\Session001\raw026.spc

GD (soman nerve agent)	Session001; scan026; match=GD (soman nerve agent) (>99.9%) 'LRD #' 'component' 'U00FXL3' 'GD (soman nerve agent)'

\\FDEC1602_ROOT\FDEC1602\20050418\History\Session001\raw027.spc

GD (soman nerve agent)	Session001; scan027; match=GD (soman nerve agent) (>99.9%) 'LRD #' 'component' 'U00FXL3' 'GD (soman nerve agent)'

SESSION 002

\\FDEC1602_ROOT\FDEC1602\20050418\History\Session002\raw001.spc

L (lewisite blister agent)	Session002; scan001; match= NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND

\\FDEC1602_ROOT\FDEC1602\20050418\History\Session002\raw002.spc

L (lewisite blister agent)	Session002; scan002; match= NO PLAUSIBLE LIBRARY MATCH FOUND MATERIAL ADDED TO LIBRARY

\\FDEC1602_ROOT\FDEC1602\20050418\History\Session002\raw003.spc

L (lewisite blister agent)	Session002; scan003; match=L (lewisite blister agent) (>99.9%) 'LRD #' 'component' 'U0243HV' 'L (lewisite blister agent)'

\\FDEC1602_ROOT\FDEC1602\20050418\History\Session002\raw004.spc

L (lewisite blister agent)	Session002; scan004; match=L (lewisite blister agent) (>99.9%) 'LRD #' 'component' 'U0243HV' 'L (lewisite blister agent)'

\\FDEC1602_ROOT\FDEC1602\20050418\History\Session002\raw005.spc

L (lewisite blister agent)	Session002; scan005; match=L (lewisite blister agent) (>99.9%) 'LRD #' 'component' 'U0243HV' 'L (lewisite blister agent)'

\\FDEC1602_ROOT\FDEC1602\20050418\History\Session002\raw006.spc

GF (cyclosarin nerve agent)	Session002; scan006; match= NO PLAUSIBLE LIBRARY MATCH FOUND MATERIAL ADDED TO LIBRARY

\\FDEC1602_ROOT\FDEC1602\20050418\History\Session002\raw007.spc

GF (cyclosarin nerve agent)	Session002; scan007; match= GF (cyclosarin nerve agent) (>99.9%) 'LRD #' 'component' 'U00MWYO' ' GF (cyclosarin nerve agent)'

\\FDEC1602_ROOT\FDEC1602\20050418\History\Session002\raw008.spc	
GF (cyclosarin nerve agent)	Session002; scan008; match= GF (cyclosarin nerve agent) (>99.9%) 'LRD #' 'component' 'U00MWYO' ' GF (cyclosarin nerve agent)'
\\FDEC1602_ROOT\FDEC1602\20050418\History\Session002\raw009.spc	
GF (cyclosarin nerve agent)	Session002; scan009; match= GF (cyclosarin nerve agent) (>99.9%) 'LRD #' 'component' 'U00MWYO' ' GF (cyclosarin nerve agent)'
\\FDEC1602_ROOT\FDEC1602\20050418\History\Session002\raw010.spc	
HN1 (nitrogen mustard)	Session002; scan010; match=2 PLAUSIBLE MATCHES FOUND (total 99.8% posterior) 'LRD #' 'component' 'U03M4KS' 'HN1 (nitrogen mustard)' 'U005P45' 'HN3 (nitrogen mustard)'

SESSION 003

\\FDEC1602_ROOT\FDEC1602\20050418\History\Session003\raw001.spc	
JP8 jet fuel	Session003; scan001; match= NO PLAUSIBLE LIBRARY MATCH FOUND MATERIAL ADDED TO LIBRARY
\\FDEC1602_ROOT\FDEC1602\20050418\History\Session003\raw002.spc	
JP8 jet fuel	Session003; scan002; match= 2 PLAUSIBLE MATCHES FOUND (total 95.7% posterior) 'LRD #' 'component' 'U00163S' 'JP8 jet fuel' 'A0278' 'Diesel #2'
\\FDEC1602_ROOT\FDEC1602\20050418\History\Session003\raw003.spc	
Butchers floor wax	Session003; scan003; match= NO PLAUSIBLE LIBRARY MATCH FOUND MATERIAL ADDED TO LIBRARY

\\FDEC1602_ROOT\FDEC1602\20050418\History\Session003\raw004.spc

Butchers floor wax	Session003; scan004; match=Butchers floor wax (>99.9%) 'LRD #' 'component' 'U03D80D' 'Butchers floor wax'

\\FDEC1602_ROOT\FDEC1602\20050418\History\Session003\raw005.spc

AFFF (aqueous film forming foam)	Session003; scan005; match=NO PLAUSIBLE LIBRARY MATCH FOUND MATERIAL ADDED TO LIBRARY

2005-04-19

SESSION 001
all SERS work

SESSION 002
Case 15 is only non-SERS work (pure VX)

\\FDEC1602_ROOT\FDEC1602\20050419\History\Session002\raw015.spc

VX (nerve agent)	Session002; scan015; match=VX (nerve agent) (>99.9%) 'LRD #' 'component' 'U021XKJ' 'VX (nerve agent)'

SESSION 003
Cases 1-3 were SERS work

\\FDEC1602_ROOT\FDEC1602\20050419\History\Session003\raw004.spc
VX not readily miscible in Windex; shaken vigorously prior to measurement

50% VX / 50% Windex	Session003; scan004; match=NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND +++++ MIXTURE ANALYSIS +++++ LIBRARY RECORD_____RECOVERY_____ VX (nerve agent) Triphenyl phosphate

\\FDEC1602_ROOT\FDEC1602\20050419\History\Session003\raw005.spc
VX immiscible; unclear which layer is VX

50% VX / 50% Windex	Session003; scan005; match=VX (nerve agent) (>99.9%) 'LRD #' 'component' 'U021XKJ' 'VX (nerve agent)'

\\FDEC1602_ROOT\FDEC1602\20050419\History\Session003\raw006.spc
VX not readily miscible in Windex; shaken vigorously prior to measurement

25% VX / 75% Windex	Session003; scan006; match=NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND +++++ MIXTURE ANALYSIS +++++ LIBRARY RECORD_____RECOVERY_____ VX (nerve agent) 2-Propanol

\\FDEC1602_ROOT\FDEC1602\20050419\History\Session003\raw007.spc
VX not readily miscible in Windex; shaken vigorously prior to measurement

25% VX / 75% Windex	Session003; scan007; match=NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND +++++ MIXTURE ANALYSIS +++++ LIBRARY RECORD_____RECOVERY_____ 2-Propanol VX (nerve agent) 2-Heptanone

\\FDEC1602_ROOT\FDEC1602\20050419\History\Session003\raw008.spc
VX not readily miscible in Windex; shaken vigorously prior to measurement

25% VX / 75% Windex	Session003; scan008; match=NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND +++++ MIXTURE ANALYSIS +++++ LIBRARY RECORD_____RECOVERY_____ VX (nerve agent) 2-Propanol

\\FDEC1602_ROOT\FDEC1602\20050419\History\Session003\raw009.spc

10% VX / 90% Windex	Session003; scan009; match= NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND +++++ MIXTURE ANALYSIS +++++ LIBRARY RECORD_____RECOVERY_____ 2-Propanol 2,6-Di-tert-butyl-4-methylphenol

\\FDEC1602_ROOT\FDEC1602\20050419\History\Session003\raw010.spc

5% VX / 95% Windex	Session003; scan010; match= NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND +++++ MIXTURE ANALYSIS +++++ LIBRARY RECORD_____RECOVERY_____ 2-Propanol

\\FDEC1602_ROOT\FDEC1602\20050419\History\Session003\raw011.spc

2.5% VX / 97.5% Windex	Session003; scan011; match= NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND +++++ MIXTURE ANALYSIS +++++ LIBRARY RECORD_____RECOVERY_____ 2-Propanol

\\FDEC1602_ROOT\FDEC1602\20050419\History\Session003\raw012.spc

1.25% VX / 98.75% Windex	Session003; scan012; match= NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND +++++ MIXTURE ANALYSIS +++++ LIBRARY RECORD_____RECOVERY_____ 2-Propanol

\\FDEC1602_ROOT\FDEC1602\20050419\History\Session003\raw013.spc
GA not readily miscible in Windex at 50%; shaken vigorously prior to measurement

50% GA / 50% Windex	Session003; scan013; match=GA (tabun nerve agent) (0.1168) 'LRD #' 'component' 'U048DAT' 'GA (tabun nerve agent)'

\\FDEC1602_ROOT\FDEC1602\20050419\History\Session003\raw014.spc
GA not readily miscible in Windex at 25%; shaken vigorously prior to measurement

25% GA / 75% Windex	Session003; scan014; match=NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND +++++ MIXTURE ANALYSIS +++++ LIBRARY RECORD_____RECOVERY_____ GA (tabun nerve agent)

\\FDEC1602_ROOT\FDEC1602\20050419\History\Session003\raw015.spc

12.5% GA / 87.5% Windex	Session003; scan015; match=NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND +++++ MIXTURE ANALYSIS +++++ LIBRARY RECORD_____RECOVERY_____ GA (tabun nerve agent) 2-Propanol

SESSION 001

\\FDEC1602_ROOT\FDEC1602\20050420\History\Session001\raw001.spc

6.25% GA / 93.75% Windex

Session001; scan001; match=NO PLAUSIBLE LIBRARY MATCH FOUND
'LRD #' 'component'
NO PLAUSIBLE LIBRARY MATCH FOUND

+++++ MIXTURE ANALYSIS +++++

LIBRARY
RECORD_____RECOVERY_____

2-Propanol
Dodecane

\\FDEC1602_ROOT\FDEC1602\20050420\History\Session001\raw002.spc

3.125% GA / 96.875% Windex

Session001; scan002; match= NO PLAUSIBLE LIBRARY MATCH FOUND
'LRD #' 'component'
NO PLAUSIBLE LIBRARY MATCH FOUND

+++++ MIXTURE ANALYSIS +++++

LIBRARY
RECORD_____RECOVERY_____

2-Propanol
2-Octanol

\\FDEC1602_ROOT\FDEC1602\20050420\History\Session001\raw003.spc
Upon mixing became white gel/solid mass

50% GA / 50% butchers floor wax

Session001; scan003; match= NO PLAUSIBLE LIBRARY MATCH FOUND

'LRD #' 'component'
NO PLAUSIBLE LIBRARY MATCH FOUND

+++++ MIXTURE ANALYSIS +++++

LIBRARY
RECORD_____RECOVERY_____

GA (tabun nerve agent)
Cluster:
Polystyrene
butchers floor wax

\\FDEC1602_ROOT\FDEC1602\20050420\History\Session001\raw004.spc
Immiscible, shaken vigorously prior to measurement

50% GA / 50% JP8 jet fuel	Session001; scan004; match=GA (tabun nerve agent) (>99.9%) 'LRD #' 'component' 'U048DAT' 'GA (tabun nerve agent)'

\\FDEC1602_ROOT\FDEC1602\20050420\History\Session001\raw005.spc
Immiscible, shaken vigorously prior to measurement

50% GA / 50% AFFF	Session001; scan005; match=GA (tabun nerve agent) (>99.9%) 'LRD #' 'component' 'U048DAT' 'GA (tabun nerve agent)'

\\FDEC1602_ROOT\FDEC1602\20050420\History\Session001\raw006.spc
White solid mass after mixing

25% GA / 75% butchers floor wax	Session001; scan006; match= NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND +++++ MIXTURE ANALYSIS +++++ LIBRARY RECORD_____RECOVERY_____ Cluster: Polystyrene butchers floor wax GA (tabun nerve agent)

\\FDEC1602_ROOT\FDEC1602\20050420\History\Session001\raw007.spc

25% GA / 75% JP8 jet fuel	Session001; scan007; match=GA (tabun nerve agent) (>99.9%) 'LRD #' 'component' 'U048DAT' 'GA (tabun nerve agent)'

\\FDEC1602_ROOT\FDEC1602\20050420\History\Session001\raw008.spc

25% GA / 75% AFFF	Session001; scan008; match= NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND +++++ MIXTURE ANALYSIS +++++ LIBRARY RECORD_____RECOVERY_____ GA (tabun nerve agent) Allyl Chloride

\\FDEC1602_ROOT\FDEC1602\20050420\History\Session001\raw009.spc

12.5% GA / 87.5%
butchers floor wax

Session001; scan009; match= NO PLAUSIBLE LIBRARY MATCH FOUND
'LRD #' 'component'
NO PLAUSIBLE LIBRARY MATCH FOUND
+++++ MIXTURE ANALYSIS +++++

LIBRARY
RECORD_____RECOVERY_____

Cluster:
Polystyrene
butchers floor wax

\\FDEC1602_ROOT\FDEC1602\History\Session001\raw010.spc

12.5% GA / 87.5%
JP8 jet fuel

Session001; scan010; match=GA (tabun nerve agent) (>99.9%)
'LRD #' 'component'
'U048DAT' 'GA (tabun nerve agent)'

\\FDEC1602_ROOT\FDEC1602\20050420\History\Session001\raw011.spc

12.5% GA / 87.5%
AFFF

Session001; scan011; match= NO PLAUSIBLE LIBRARY MATCH FOUND
'LRD #' 'component'
NO PLAUSIBLE LIBRARY MATCH FOUND
+++++ MIXTURE ANALYSIS +++++
LIBRARY
RECORD_____RECOVERY_____

GA (tabun nerve agent)
Cluster:
Polystyrene
butchers floor wax

\\FDEC1602_ROOT\FDEC1602\20050420\History\Session001\raw012.spc

6.25% GA / 93.75%
AFFF

Session001; scan012; match= NO PLAUSIBLE LIBRARY MATCH FOUND

'LRD #' 'component'
NO PLAUSIBLE LIBRARY MATCH FOUND

+++++ MIXTURE ANALYSIS +++++

LIBRARY
RECORD_____RECOVERY_____

Cluster:
Polystyrene
butchers floor wax
GA (tabun nerve agent)

SESSION 002 – write to drive failure, session aborted

SESSION 003

\\FDEC1602_ROOT\FDEC1602\20050420\History\Session003\raw001.spc
VX very miscible in JP8

50% VX / 50% JP8 jet fuel	Session003; scan001; match=VX (nerve agent) (>99.9%) 'LRD #' 'component' 'U021XKJ' 'VX (nerve agent)'

\\FDEC1602_ROOT\FDEC1602\History\Session003\raw002.spc

25% VX / 75% JP8 jet fuel	Session003; scan002; match= NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND +++++ MIXTURE ANALYSIS +++++ LIBRARY RECORD_____RECOVERY_____ VX (nerve agent) Cluster: Diesel #2 JP8 (jet fuel)

\\FDEC1602_ROOT\FDEC1602\20050420\History\Session003\raw003.spc
HD very miscible in JP8

50% HD / 50% JP8 jet fuel	Session003; scan003; match=HD (mustard) (>99.9%) 'LRD #' 'component' 'U001PI1' 'HD (distilled mustard)'

\\FDEC1602_ROOT\FDEC1602\20050420\History\Session003\raw004.spc

25 % HD / 75% JP8 jet fuel	Session003; scan004; match=NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND +++++ MIXTURE ANALYSIS +++++ LIBRARY RECORD_____RECOVERY_____ HD (distilled mustard) 2-sec-Butylphenol Isobutylbenzene Cluster: Diesel #2 JP8 (jet fuel)

SESSION 004

\\FDEC1602_ROOT\FDEC1602\20050420\History\Session004\raw001.spc

50% HD / 50% AFFF	Session004; scan001; match=HD (mustard) (>99.9%) 'LRD #' 'component' 'U001PI1' 'HD (distilled mustard)'

SESSION 005

\\FDEC1602_ROOT\FDEC1602\20050420\History\Session005\raw001.spc

25% HD / 75% AFFF	Session005; scan001; match=HD (mustard) (>99.9%) 'LRD #' 'component' 'U001PI1' 'HD (distilled mustard)'

\\FDEC1602_ROOT\FDEC1602\20050420\History\Session005\raw002.spc

25% HD / 75% AFFF	Session005; scan002; match=HD (mustard) (>99.9%) 'LRD #' 'component' 'U001PI1' 'HD (distilled mustard)'

\\FDEC1602_ROOT\FDEC1602\20050420\History\Session005\raw003.spc
GB somewhat miscible in JP8

50% GB / 50% JP8 jet fuel	Session005; scan003; match=GB (sarin nerve agent) (>99.9%) 'LRD #' 'component' 'U03JO2U' 'GB (sarin nerve agent)'

\\FDEC1602_ROOT\FDEC1602\20050420\History\Session005\raw004.spc

25% GB / 75% JP8 jet fuel	Session005; scan004; match=NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND +++++ MIXTURE ANALYSIS +++++ LIBRARY RECORD_____RECOVERY_____ GB (sarin nerve agent)

\\FDEC1602_ROOT\FDEC1602\20050420\History\Session005\raw005.spc

25% GB / 75% JP8 jet fuel	Session005; scan005; match=NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND +++++ MIXTURE ANALYSIS +++++ LIBRARY RECORD_____RECOVERY_____ GB (sarin nerve agent)

\\FDEC1602_ROOT\FDEC1602\20050420\History\Session005\raw006.spc

25% GB / 75% JP8 jet fuel	Session005; scan006; match= NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND +++++ MIXTURE ANALYSIS +++++ LIBRARY RECORD_____RECOVERY_____ GB (sarin nerve agent)

\\FDEC1602_ROOT\FDEC1602\20050420\History\Session005\raw007.spc
GB seems miscible with Windex

50% GB / 50% Windex	Session005; scan007; match=GB (sarin nerve agent) (>99.9%) 'LRD #' 'component' 'U03JO2U' 'GB (sarin nerve agent)'

\\FDEC1602_ROOT\FDEC1602\20050420\History\Session005\raw008.spc

25% GB / 75% Windex	Session005; scan008; match=GB (sarin nerve agent) (>99.9%) 'LRD #' 'component' 'U03JO2U' 'GB (sarin nerve agent)'

\\FDEC1602_ROOT\FDEC1602\20050420\History\Session005\raw009.spc

12.5% GB / 87.5% Windex	Session005; scan009; match=NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND +++++ MIXTURE ANALYSIS +++++ LIBRARY RECORD_____RECOVERY_____ GB (sarin nerve agent) Choline chloride Dipentene 4-Methylanisole

\\FDEC1602_ROOT\FDEC1602\20050420\History\Session005\raw010.spc
GB seems miscible in AFFF

50% GB / 50% AFFF

Session005; scan010; match=GB (sarin nerve agent) (99.6%)

'LRD #' 'component'
'U03JO2U' 'GB (sarin nerve agent)'

\\FDEC1602_ROOT\FDEC1602\20050420\History\Session005\raw011.spc

25% GB / 75% AFFF

Session005; scan011; match=NO PLAUSIBLE LIBRARY MATCH FOUND

'LRD #' 'component'
NO PLAUSIBLE LIBRARY MATCH FOUND

+++++ MIXTURE ANALYSIS +++++

LIBRARY
RECORD_____RECOVERY_____

GB (sarin nerve agent)
Acetone

\\FDEC1602_ROOT\FDEC1602\20050420\History\Session005\raw012.spc
GD seems miscible with JP8

50% GD / 50% JP8 jet fuel

Session005; scan012; match=GD (soman nerve agent) (>99.9%)

'LRD #' 'component'
'U00FXL3' 'GD (soman nerve agent)'

\\FDEC1602_ROOT\FDEC1602\20050420\History\Session005\raw013.spc

25% GD / 75% Windex

Session005; scan013; match=NO PLAUSIBLE LIBRARY MATCH FOUND

'LRD #' 'component'
NO PLAUSIBLE LIBRARY MATCH FOUND

+++++ MIXTURE ANALYSIS +++++

LIBRARY
RECORD_____RECOVERY_____

GD (soman nerve agent)
2-Propanol
Teflon

\\FDEC1602_ROOT\FDEC1602\20050420\History\Session005\raw014.spc

	Session005; scan014; match=NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND
50% GD / 50% Windex	+++++ MIXTURE ANALYSIS +++++ LIBRARY RECORD_____RECOVERY_____ GD (soman nerve agent)

\\FDEC1602_ROOT\FDEC1602\20050420\History\Session005\raw015.spc

	Session005; scan015; match=NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND
12.5% GD / 87.5% Windex	+++++ MIXTURE ANALYSIS +++++ LIBRARY RECORD_____RECOVERY_____ GD (soman nerve agent)

2005-04-21

SESSION 001

\\FDEC1602_ROOT\FDEC1602\20050421\History\Session001\raw001.spc
L seems miscible in JP8; solution took on a rose color

	Session001; scan001; match=NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND
50% L / 50% JP8 jet fuel	+++++ MIXTURE ANALYSIS +++++ LIBRARY RECORD_____RECOVERY_____ L (lewisite blister agent) +86.5604% (Cumulative 86.5604%) 1-Butanol 2-Mercaptobenzothiazole Anthracene

\\FDEC1602_ROOT\FDEC1602\20050421\History\Session001\raw002.spc
Polystyrene check sample

polystyrene	Session001; scan002; match=Polystyrene (>99.9%) 'LRD #' 'component' 'A0001' 'Polystyrene'

\\FDEC1602_ROOT\FDEC1602\20050421\History\Session001\raw003.spc

50% L / 50% JP8 jet fuel	Session001; scan003; match= NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND +++++ MIXTURE ANALYSIS +++++ LIBRARY RECORD_____RECOVERY_____ L (lewisite blister agent) +102.4699% (Cumulative 102.4699%) Anthracene

\\FDEC1602_ROOT\FDEC1602\20050421\History\Session001\raw004.spc

50% L / 50% JP8 jet fuel	Session001; scan004; match= NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND +++++ MIXTURE ANALYSIS +++++ LIBRARY RECORD_____RECOVERY_____ L (lewisite blister agent) +113.7798% (Cumulative 113.7798%) 2-Mercaptobenzothiazole Anthracene Ethyl acrylate

\\FDEC1602_ROOT\FDEC1602\20050421\History\Session001\raw005.spc
Seem to be miscible

50% HN3 / 50% JP8 jet fuel	Session001; scan005; match=2 PLAUSIBLE MATCHES FOUND (total 97.8% posterior) 'LRD #' 'component' 'U03M4KS' 'HN1 (nitrogen mustard)' 'U005P45' 'HN3 (nitrogen mustard)'

\\FDEC1602_ROOT\FDEC1602\20050421\History\Session001\raw006.spc

25% HN3 / 75% JP8 jet fuel	Session001; scan006; match=NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND +++++ MIXTURE ANALYSIS +++++ LIBRARY RECORD_____RECOVERY_____ Cluster: HN-1 (nitrogen mustard blister agent) HN-3 (nitrogen mustard blister agent) AFFF tert-Butyl methyl ether

\\FDEC1602_ROOT\FDEC1602\20050421\History\Session001\raw007.spc
Mixture turned milky light blue color, somewhat miscible

50% HN3 / 50% Windex	Session001; scan007; match=2 PLAUSIBLE MATCHES FOUND (total 95.5%) 'LRD #' 'component' 'U03M4KS' 'HN1 (nitrogen mustard)' 'U005P45' 'HN3 (nitrogen mustard)'

\\FDEC1602_ROOT\FDEC1602\20050421\History\Session001\raw008.spc

25% HN3 / 75% Windex	Session001; scan008; match=2 PLAUSIBLE MATCHES FOUND (total 99.6% posterior) 'LRD #' 'component' 'U03M4KS' 'HN1 (nitrogen mustard)' 'U005P45' 'HN3 (nitrogen mustard)'

\\FDEC1602_ROOT\FDEC1602\20050421\History\Session001\raw009.spc
Milky light blue mixture, somewhat miscible

50% HN3 / 50% AFFF	Session001; scan009; match=2 PLAUSIBLE MATCHES FOUND (total 99.9% posterior) 'LRD #' 'component' 'U005P45' 'HN3 (nitrogen mustard)' 'U03M4KS' 'HN1 (nitrogen mustard)'

\\FDEC1602_ROOT\FDEC1602\20050421\History\Session001\raw010.spc
Solid particulate present, two layers milky on the bottom, somewhat miscible

25% HN3 / 75% AFFF	Session001; scan010; match=2 PLAUSIBLE MATCHES FOUND (total >99.9% posterior) 'LRD #' 'component' 'U005P45' 'HN3 (nitrogen mustard)' 'U03M4KS' 'HN1 (nitrogen mustard)'

\\FDEC1602_ROOT\FDEC1602\20050421\History\Session001\raw011.spc

Neat VX (nerve agent)	Session001; scan011; match=VX (nerve agent) (>99.9%) 'LRD #' 'component' 'U021XKJ' 'VX (nerve agent)'

\\FDEC1602_ROOT\FDEC1602\20050421\History\Session001\raw012.spc

Neat L (lewisite)	Session001; scan012; match=L (lewisite blister agent) (>99.9%) 'LRD #' 'component' 'U0243HV' 'L (lewisite blister agent)'

\\FDEC1602_ROOT\FDEC1602\20050421\History\Session001\raw013.spc
Somewhat miscible, two layers evident

66% L / 33% AFFF	Session001; scan013; match=L (lewisite blister agent) (>99.9%) 'LRD #' 'component' 'U0243HV' 'L (lewisite blister agent)'

\\FDEC1602_ROOT\FDEC1602\20050421\History\Session001\raw014.spc

50% L / 50% AFFF	Session001; scan014; match=L (lewisite blister agent) (>99.9%) 'LRD #' 'component' 'U0243HV' 'L (lewisite blister agent)'

\\FDEC1602_ROOT\FDEC1602\20050421\History\Session001\raw015.spc

	Session001; scan015; match=NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND
25% L / 75% AFFF	+++++ MIXTURE ANALYSIS +++++ LIBRARY RECORD_____RECOVERY_____ L (lewisite blister agent) +93.4771% (Cumulative 93.4771%)

\\FDEC1602_ROOT\FDEC1602\20050421\History\Session001\raw016.spc
Sparingly miscible, Windex appears to be supernatant

	Session001; scan016; match=NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND
50% L / 50% Windex	+++++ MIXTURE ANALYSIS +++++ LIBRARY RECORD_____RECOVERY_____ L (lewisite blister agent) +95.0594% (Cumulative 95.0594%) Pentachloronitrobenzene

\\FDEC1602_ROOT\FDEC1602\20050421\History\Session001\raw017.spc

	Session001; scan017; match=NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND
25% L / 75% Windex	+++++ MIXTURE ANALYSIS +++++ LIBRARY RECORD_____RECOVERY_____ L (lewisite blister agent) +72.4721% (Cumulative 72.4721%) Pentachloronitrobenzene 2-Amino-2-methyl-1-propanol

\\FDEC1602_ROOT\FDEC1602\20050421\History\Session001\raw018.spc
Sample also contained 5% AFFF due to technician mix-up

25% L / 75% JP8 jet fuel	Session001; scan018; match=NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND +++++ MIXTURE ANALYSIS +++++ NO PLAUSIBLE MIXTURE SOLUTION

\\FDEC1602_ROOT\FDEC1602\20050421\History\Session001\raw019.spc
Resulting mixture was milky yellow; solid particulate evident

50% VX / 50% JP8 jet fuel	Session001; scan019; match=NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND +++++ MIXTURE ANALYSIS +++++ LIBRARY RECORD_____RECOVERY_____ VX (nerve agent) Cluster: Diesel #2 JP8 (jet fuel)

\\FDEC1602_ROOT\FDEC1602\20050421\History\Session001\raw020.spc

25% VX / 75% JP8 jet fuel	Session001; scan020; match=NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND +++++ MIXTURE ANALYSIS +++++ LIBRARY RECORD_____RECOVERY_____ VX (nerve agent) Cluster: Diesel #2 JP8 (jet fuel)

\\FDEC1602_ROOT\FDEC1602\20050421\History\Session001\raw021.spc

50% VX / 50% AFFF

Session001; scan021; match= NO PLAUSIBLE LIBRARY MATCH FOUND

'LRD #' 'component'
NO PLAUSIBLE LIBRARY MATCH FOUND

+++++ MIXTURE ANALYSIS +++++

LIBRARY
RECORD_____RECOVERY_____

VX (nerve agent)

\\FDEC1602_ROOT\FDEC1602\20050421\History\Session001\raw022.spc

25% VX / 75% AFFF

Session001; scan022; match= NO PLAUSIBLE LIBRARY MATCH FOUND

'LRD #' 'component'
NO PLAUSIBLE LIBRARY MATCH FOUND

+++++ MIXTURE ANALYSIS +++++

LIBRARY
RECORD_____RECOVERY_____

Dimethyl sulfoxide
Dichlorodimethylsilane
m-Xylene
N,N-Dimethylacetamide

\\FDEC1602_ROOT\FDEC1602\20050421\History\Session001\raw023.spc

50% GD / 50% AFFF

Session001; scan023; match=GD (soman nerve agent) (>99.9%)

'LRD #' 'component'
'U00FXL3' 'GD (soman nerve agent)'

\\FDEC1602_ROOT\FDEC1602\20050421\History\Session001\raw024.spc

25% GD / 75% AFFF	Session001; scan024; match=NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND +++++ MIXTURE ANALYSIS +++++ LIBRARY RECORD_____RECOVERY_____ GD (soman nerve agent)

\\FDEC1602_ROOT\FDEC1602\20050421\History\Session001\raw025.spc

12.5% GD / 87.5% AFFF	Session001; scan025; match=NO PLAUSIBLE LIBRARY MATCH FOUND 'LRD #' 'component' NO PLAUSIBLE LIBRARY MATCH FOUND +++++ MIXTURE ANALYSIS +++++ LIBRARY RECORD_____RECOVERY_____ GD (soman nerve agent) Cluster: Polystyrene butchers floor wax